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Nonequilibrium thermodynamics approach to the mesomechanics of a deformed solid as a multiscale system

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Abstract

Based on non-equilibrium thermodynamics, we develop a methodology of describing a deformed solid as a multiscale system. It is concluded that all mechanisms of plastic deformation and fracture of solids as local structural transformations in the zones of stress concentrators of different scales are common in nature. All types of strain-induced defects are generated in hydrostatic tension zones near stress concentrators, where the local non-equilibrium thermodynamic Gibbs potential should be considered. The corpuscular-wave dualism of plastic shear is demonstrated and its specific character at different structural scale levels of plastic deformation is shown.

Keywords: physical mesomechanics, deformation, strain-induced defects, scale levels, thermodynamic approach

1. Introduction

All kinds of stress-induced damage in a crystal under loading are linked to local structural or structural-phase transformations. In open hierarchical systems they should be described on the basis of the thermodynamics of non-equilibrium processes with regard to local effective fields in different-scale hydrostatic tension zones. Local potentials $u(v, \alpha)$ related to effective fields in the hydrostatic tension zones are introduced for the dependence of the thermodynamics Gibbs potential $F(v, \alpha)$ on molar volume v. The local structural transformations occur in these zones, which locally reduce the thermodynamic Gibbs potential due to entropy production. The system approach based on the description of local thermodynamic potentials and on the Gibbs method in open hierarchical systems allows representing all-type of strain-induced defects, including cracks, in terms of local structural transformations.

2. Methodology of multiscale description of nonequilibrium thermodynamics

Estimation of the "effective potential" $u(v, \alpha)$ in the hydrostatic tension zones can be made using the theory of entropy production, σ_s, related to local structural transformations. Equation for σ_s is of the form [1]:

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$$\sigma_s = \frac{\chi(\nabla T)^2}{T^2} + \rho\frac{\bar{v}\bar{\sigma}}{T} - \frac{\rho}{T^2}([\bar{\alpha}\bar{v}],\nabla T), \quad (1)$$

where χ is the heat conductivity, T is the temperature, $\bar{\alpha}$ is the defect density, $\bar{v}$ is a quantity proportional to the defect flow density and $\bar{\sigma}$ is the applied stress. The first term in (1) is related to the heat release. The second term is due to the work of defect flow in the hydrostatic tension zone and the third one expresses the flow of the mechanical field energy through the plastic shear front.

According to (1), the dependence of the thermodynamic Gibbs potential on molar volume, v, is of the form represented in Fig.1.

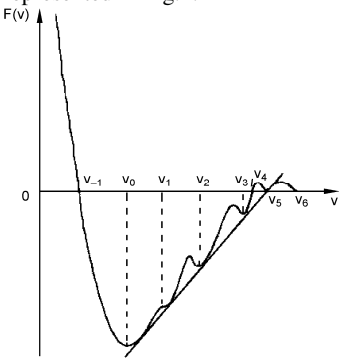

Fig. 1. Variations of the Gibbs thermodynamic potential $F(v)$ with a molar volume v having regard to local zones of hydrostatic tension of different scales where local structural or structural-phase transformations of different scales and structural-phase decomposition for $F(v) > 0$ can take place

At critical values of the molar volume v_i (i = 1, 2, …, 6), the thermodynamic potential $F(v_i, \alpha)$ passes through local minima that reflect local non-equilibrium potentials in different-scale hydrostatic tension zones. The critical values correspond to the following states in the deformed solid:

a. v_{-1} — $F(v, \alpha)$ changes from negative to positive under hydrostatic compression;
b. v_0 — equilibrium crystal;
c. v_1 — stress microconcentrator zones where dislocation cores are generated;
d. v_2, v_3 — stress meso- and macroconcentrator zones where local structural phase transitions occur with the formation of meso- and macrobands of localized plastic deformation, respectively;
e. v_4 corresponds to the intersection of the curve $F(v, \alpha)$ with the abscissa; with further expansion of the local molar volume, the thermodynamic Gibbs potential becomes positive and the system unstable: different types of material destruction take place in this condition;
f. at $v > v_4$ two phases may coexist: nanocluster quasi-amorphous phase (at $v = v_5$) and local vacuum (at $v \geq v_6$) in the form of micropores, cracks and discontinuities;
g. as evident from Fig. 1, all local minima in the curve $F(v_i)|_{i=1}^{5}$ have common conodes with the major minimum of the equilibrium thermodynamic potential at $v = v_0$. This means that a non-deformed equilibrium medium should always remain in the deformed solid at plastic strain localization in which all kinds of strain-induced defects, including unstable quasi-amorphous phases, may coexist.

With such thermodynamic representation of the $F(v)$ curve stages in Fig. 1, the following stages of deformation and fracture of the loaded solid can be assigned to them:

- stage $v < v_{-1}$ corresponds to hydrostatic compression and is characterized by incompressibility of the solid.
- $v_{-1} - v_1$ — stage of elastic compression-tension of an equilibrium crystal;
- $v_1 - v_4$ — stage of plastic deformation of the solid without signs of destruction in the defect-containing material; at this stage, the equilibrium state of the material can be completely recovered (e.g., at annealing);
- $v_4 - v_6$ — stage where different-scale discontinuities, micropores and cracks, are generated; viscous flow and sublimation of the material in the solid state are possible;

Under an inhomogeneous stress-strain state (compression + torsion in Bridgman anvils, equal channel angular pressing, etc.), material fragmentation takes place where submicro/nanofragments of the equilibrium material are surrounded by layers of the non-equilibrium quasi-amorphous phase, Fig. 2. This process is central to the production of submicro/nanostructured materials under severe plastic deformation. In the given stage of highly non-equilibrium states, explosive fragmentation is also possible (e.g., in passing high-power current pulses through the material).

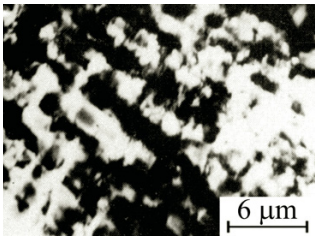

Fig. 2. Two systems of band structures along the conjugate directions of maximum tangential stresses at the stage of band structure degradation and material fragmentation. Steel Cr20NMn20V; cold rolling at 293 K, ε = 95 %

3. Corpuscular – wave dualism of plastic deformation of solids

In solid state physics and solid mechanics, the plastic deformation of solids is conventionally described on the basis of the linear approaches of Newton's mechanics. Force models of plastic shear evolution are central to the approaches. At the same time, a nonlinear approach for describing plastic deformation is developed on the basis of the continuum theory of strain-induced defects. It predicts the wave evolution of plastic shears [2, 3]. It can be shown that within the multiscale approach the nature of any plastic shears is related to their corpuscular-wave dualism.

Paper [4], by analogy with electrodynamics, puts forward the following system of wave equations for the dimensionless values of the strain-induced defect density, α, and their flux, J, (which are determined by the discontinuity of displacement vector u):

$$\frac{\partial}{\partial x_\alpha} J_\mu^\alpha = -\frac{\partial \ln u_\mu}{\partial t}, \tag{2}$$

$$\varepsilon_{\mu\chi\delta} \frac{\partial J_\delta^\alpha}{\partial x_\chi} = -\frac{\partial \alpha_\mu^\alpha}{\partial t}, \tag{3}$$

$$\frac{\partial \alpha_\mu^\alpha}{\partial x_\alpha} = 0, \tag{4}$$

$$\varepsilon_{\mu\chi\delta} \frac{\partial \alpha_\delta^\alpha}{\partial x_\chi} = \frac{1}{\tilde{c}^2} \frac{\partial J_\mu^\alpha}{\partial t} + \sigma_\mu^\alpha - P_\mu^\beta \frac{C_{\alpha\beta}^{\mu\nu}}{E}, \tag{5}$$

$$\frac{1}{c^2} \frac{\partial v_\mu}{\partial t} = \frac{\partial \sigma_\mu^\alpha}{\partial x_\alpha} - \frac{\partial P_\nu^\beta C_{\alpha\beta}^{\mu\nu}}{\partial x_\alpha E}, \tag{6}$$

where $v_\mu = \frac{\partial \ln u_\mu}{\partial t}$ is the elastic strain rate of a medium with defects, $\sigma_\mu^\alpha = \frac{\partial \ln u_\nu}{\partial x_\beta} \frac{C_{\alpha\beta}^{\mu\nu}}{E}$ are the elastic stresses in the medium, c and $\tilde{c}$ are respectively the sound velocity and velocity of the plastic perturbation front, $P_\alpha^\mu(x,t)$ is the plastic part of distortion, $\varepsilon_{\mu\chi\delta}$ is the Levi-Civita symbol, and $C_{\alpha\beta}^{\mu\nu}$ are the elastic constants.

Using the system of equations (2)–(6) we can derive the wave equations for the dimensionless values of the flux J and the defect density α as follows:

$$\frac{1}{c^2} \frac{\partial^2 J_\alpha^\mu}{\partial t^2} - \frac{\partial^2 J_\alpha^\mu}{\partial x_\nu^2} = \frac{\partial}{\partial t} \left(\frac{\partial \ln u_\alpha(x,l)}{\partial x_\mu} - \frac{1}{E} \frac{\partial \ln u_\beta}{\partial x_\nu} C_{\alpha\beta}^{\mu\nu} - \frac{1}{E} P_\nu^\beta C_{\alpha\beta}^{\mu\nu} \right), \tag{7}$$

$$\frac{1}{c^2}\frac{\partial^2\alpha_\alpha^\mu}{\partial t^2}-\frac{\partial^2\alpha_\alpha^\mu}{\partial x_\nu^2}=\varepsilon_{\mu\chi\sigma}\left\{\frac{\partial^2\ln u_\beta(x,t)}{\partial x_\chi\partial x_\nu}C_{\alpha\beta}^{\mu\nu}-\frac{\partial P_\nu^\beta}{\partial x_\chi}C_{\alpha\beta}^{\mu\nu}\right\}\frac{1}{E}. \tag{8}$$

The right side of equation (7) characterizes the sources of the defect flow. They are defined by the rate of quasi-elastic deformation $\frac{\partial}{\partial t}(E_\mu^\alpha E-E_\nu^\beta C_{\alpha\beta}^{\mu\nu})\frac{1}{E}$. The expression in brackets is the difference between the internal compressive stresses and the shear stresses related to stress distribution in the stress concentrator zone.

The relaxation processes associated with the rearrangement of defects (such as clusters of various atomic configurations or their conglomerates) are represented in (7) by the term $P_\nu^\beta C_{\alpha\beta}^{\mu\nu}/E$. The right side of equation (8) characterizes the source of strain-induced defect density. The source is presented by the vorticity, $\varepsilon_{\mu\chi\delta}\frac{\partial}{\partial x}(E_\nu^\beta-P_\nu^\beta)\frac{C_{\alpha\beta}^{\mu\nu}}{E}$, of shear deformation induced by the shear stress relaxation in local hydrostatic tension zones. The character of the wave flows of strain-induced defects is described by the right side of equations (6) and (7). The plastic distortion $P_\nu^\beta(x,t)$ plays a crucial role in the wave flow generation.

In the case of microscale dislocational deformation, the local compressive inelastic deformation in the stress micro–concentrator zone and the plastic distortion in the dislocation core make up a soliton pair. This determines a high mobility of dislocations in the conditions of thermodynamic stability of the equilibrium crystal. The related dispersion of dislocation shears is responsible for the decay of the periodic plastic flow waves at the microscale level. In equations (7) and (8) this is represented by high values of their right side.

For a thermodynamically non-equilibrium crystal, the local compressive inelastic deformation in the zones of meso- and macroscopic stress concentrators is distinguished by low amplitudes. The plastic distortion in the hydrostatic tension zone behind the stress concentrator relaxes stresses in this zone periodically, generating rotational bending-torsion modes in the stress concentrator zone simultaneously. The given process leads to the decomposition of the nonequilibrium crystal structure in extended meso- and macrobands of localized deformation. The right sides of equations (7) and (8) turn to be small and periodically oscillating. Plastic shears in the localized deformation meso- and macrobands evolve as oscillating nonlinear wave processes.

4. Conclusion

All strain-induced defects in a deformed solid are related to the structural (dislocations, disclinations) or structural-phase (meso- and macrobands of localized shear, cracks) transformations. The kind of strain-induced defects is defined by the excitation scale of the non-equilibrium thermodynamics Gibbs potential.

Local structural or structure-phase transformations can take place only in local zones of hydrostatic tension. It explains the plastic flow localization in the hierarchy of scale levels. Any plastic shear develops at nanoscale as a nonlinear-wave process of curvature soliton motion. Propagation of any stress concentrator is described by Newton's mechanics. The combination of Newton's mechanics and physics of local structural – phase transformations defines the corpuscular-wave dualism of plastic shear.

Failure of a solid under loading takes place when non-equilibrium thermodynamic potential $F(v, \alpha)$ becomes positive in local zones of hydrostatic tension where highly excited non-equilibrium states arise and crystal lattice undergoes structural-phase decomposition.

References

1. Panin VE (ed.) *Physical mesomechanics of heterogeneous media and computer-aided design of materials*. Cambridge; Cambridge Interscience Publishing: 1998

2. Panin VE, Grinyaev YuV, Egorushkin VE et al. Excited state spectrum and vortex mechanical field in a deformable crystal. *Russ Phys J* 1987; **30:** 1-34.

3. Infeld E and Rowlands G. *Nonlinear Waves,Ssolitons and Chaos*. Cambridge: Cambridge University Press: 2000.

4. Egorushkin VE. Dinamics of plastic deformation. Waves of localized plastic deformation in solids. *Russ Phys J* 1992; **35**: 4-316.